

1,4-Dideoxy-1,4-iminothreitol
90481-32-6 | DTXSID50238179

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: -2.10

Global applicability domain: Inside

Local applicability domain index: 5.26e-01

Confidence level: 7.04e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Diethanolamine</div> <div>Measured: -1.43</div> <div>Predicted: -1.46</div>	<div>Image not found</div> <div>L-Threonine</div> <div>Measured: -2.94</div> <div>Predicted: -2.93</div>	<div>Image not found</div> <div>Glycerol</div> <div>Measured: -1.76</div> <div>Predicted: -1.81</div>
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